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NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	SEP 09	ACD predicted properties enhanced in REGISTRY/ZREGISTRY
NEWS 4	OCT 03	MATHDI removed from STN
NEWS 5	OCT 04	CA/CAplus-Canadian Intellectual Property Office (CIPO) added to core patent offices
NEWS 6	OCT 13	New CAS Information Use Policies Effective October 17, 2005
NEWS 7	OCT 17	STN(R) AnaVist(TM), Version 1.01, allows the export/download of CAplus documents for use in third-party analysis and visualization tools
NEWS 8	OCT 27	Free KWIC format extended in full-text databases
NEWS 9	OCT 27	DIOGENES content streamlined
NEWS 10	OCT 27	EPFULL enhanced with additional content
NEWS 11	NOV 14	CA/CAplus - Expanded coverage of German academic research
NEWS 12	NOV 30	REGISTRY/ZREGISTRY on STN(R) enhanced with experimental spectral property data

NEWS EXPRESS DECEMBER 02 CURRENT VERSION FOR WINDOWS IS V8.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 02 DECEMBER 2005. V8.0 USERS CAN OBTAIN THE UPGRADE TO V8.01 AT http://download.cas.org/express/v8.0-Discover/

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:12:28 ON 02 DEC 2005

=>

Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 13:12:45 ON 02 DEC 2005

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 30 NOV 2005 HIGHEST RN 869059-01-8
DICTIONARY FILE UPDATES: 30 NOV 2005 HIGHEST RN 869059-01-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

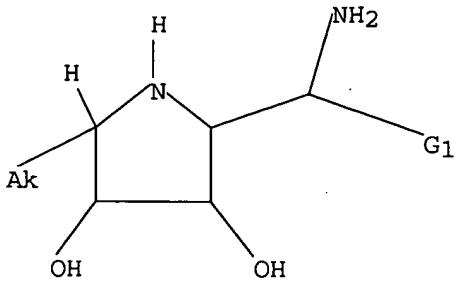
****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

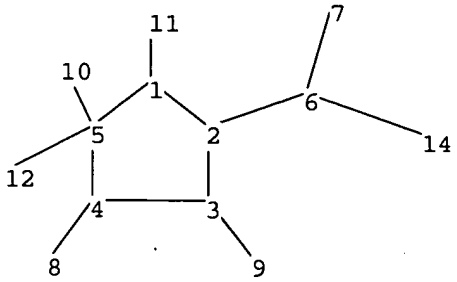
Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10726550.str





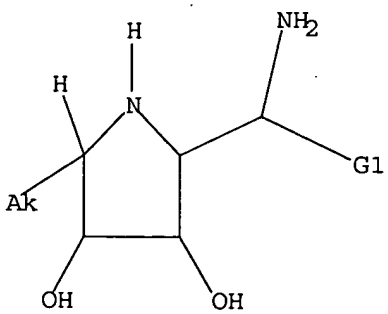
chain nodes :
6 7 8 9 10 11 12 14
ring nodes :
1 2 3 4 5
chain bonds :
1-11 2-6 3-9 4-8 5-10 5-12 6-7 6-14
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 3-9 4-8 5-12 6-7 6-14
exact bonds :
1-11 2-3 2-6 3-4 4-5 5-10
isolated ring systems :
containing 1 :

G1:H,CH2,COOH

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 14:CLASS

L1 STRUCTURE UPLOADED

=> D L1
L1 HAS NO ANSWERS
L1 STR



G1 H,CH2,COOH

Structure attributes must be viewed using STN Express query preparation.

```
=> S L1
SAMPLE SEARCH INITIATED 13:12:59 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       80 TO ITERATE

100.0% PROCESSED       80 ITERATIONS                                 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         1064 TO     2136
PROJECTED ANSWERS:               1 TO       80

L2             1 SEA SSS SAM L1

=> S L1 SSS FULL
FULL SEARCH INITIATED 13:13:05 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     1625 TO ITERATE

100.0% PROCESSED     1625 ITERATIONS                                 15 ANSWERS
SEARCH TIME: 00.00.01

L3            15 SEA SSS FUL L1

=> FIL HCAPLUS
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   161.33     161.54

FILE 'HCAPLUS' ENTERED AT 13:13:10 ON 02 DEC 2005
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FILE COVERS 1907 - 2 Dec 2005  VOL 143 ISS 24
FILE LAST UPDATED: 1 Dec 2005  (20051201/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> S L3
L4            11 L3

=> d l4 ibib abs hitstr tot

L4   ANSWER 1 OF 11  HCAPLUS  COPYRIGHT 2005 ACS on STN
```
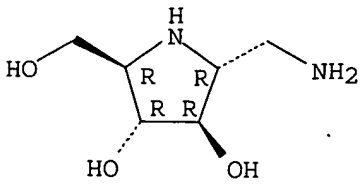

ACCESSION NUMBER: 2004:634317 HCAPLUS
DOCUMENT NUMBER: 141:314531
TITLE: Synthesis and High-Throughput Screening of N-Acetyl-β-hexosaminidase Inhibitor Libraries Targeting Osteoarthritis
AUTHOR(S): Liu, Junjie; Numa, Mehdi M. D.; Liu, Haitian; Huang, Shi-Jung; Sears, Pamela; Shikhman, Alexander R.; Wong, Chi-Huey
CORPORATE SOURCE: Department of Chemistry and the Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Journal of Organic Chemistry (2004), 69(19), 6273-6283
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB C1 Nitrogen iminocyclitols are potent inhibitors of N-acetyl-β-hexosaminidases. Given hexosaminidases' important roles in osteoarthritis, we developed two straightforward and efficient syntheses of C1 nitrogen iminocyclitols from two readily available starting materials, D-mannosamine hydrochloride and the microbial oxidation product of fructose. A diversity-oriented synthetic strategy was then performed by coupling these core structures with various aldehydes, carboxylic acids, and alkynes to generate three sep. libraries. High-throughput screening of the generated libraries with human N-acetyl-β-hexosaminidases produced only moderate inhibitory activities. However, the synthetic approach and screening strategy for these compds. will be applied to develop new potent inhibitors of human N-acetyl-β-hexosaminidases, particularly when combined with the structural information of these enzymes.

IT **194288-65-8P**
RL: CRT (Combinatorial reactant); RCT (Reactant); SPN (Synthetic preparation); CMBI (Combinatorial study); PREP (Preparation); RACT (Reactant or reagent)
(preparation and screening of iminocyclitol-deriviative N-acetyl-β-hexosaminidase inhibitors)
RN 194288-65-8 HCAPLUS
CN 3,4-Pyrrolidinediol, 2-(aminomethyl)-5-(hydroxymethyl)-, (2R,3R,4R,5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

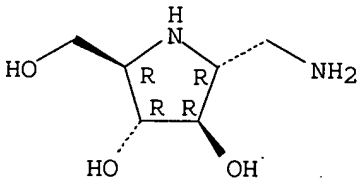
L4 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:469769 HCAPLUS
DOCUMENT NUMBER: 141:291056
TITLE: Probing the aglycon binding site of a β-glucosidase: a collection of C-1-modified 2,5-dideoxy-2,5-imino-D-mannitol derivatives and their

structure-activity relationships as competitive inhibitors
AUTHOR(S): Wrodnigg, Tanja M.; Diness, Frederik; Gruber, Christoph; Hausler, Herwig; Lundt, Inge; Rupitz, Karen; Steiner, Andreas J.; Stutz, Arnold E.; Tarling, Chris A.; Withers, Stephen G.; Wolfler, Heidrun
CORPORATE SOURCE: Glycogroup, Institut fuer Organische Chemie, Technische Universitaet Graz, Graz, A-8010, Austria
SOURCE: Bioorganic & Medicinal Chemistry (2004), 12(13), 3485-3495
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:291056

AB A range of new C-1 modified derivs. of the powerful glucosidase inhibitor 2,5-dideoxy-2,5-imino-D-mannitol has been synthesized and their biol. activities probed with the β-glucosidase from Agrobacterium sp. Ki values are compared with those of previously prepared close relatives. Findings suggest dramatic effects exerted by the aglycon binding site on substrate/inhibitor binding.

IT **194288-65-8**
RL: BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(synthesis of C-1-modified 2,5-dideoxy-2,5-imino-D-mannitol derivs.)
RN 194288-65-8 HCAPLUS
CN 3,4-Pyrrolidinediol, 2-(aminomethyl)-5-(hydroxymethyl)-, (2R,3R,4R,5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

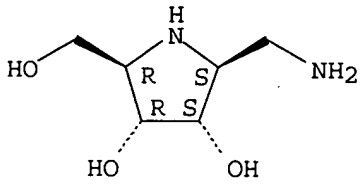
L4 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:400378 HCAPLUS
DOCUMENT NUMBER: 141:38786
TITLE: Syntheses and glycosidase inhibitory activities of 2-(aminomethyl)-5-(hydroxymethyl)pyrrolidine-3,4-diol derivatives
AUTHOR(S): Popowycz, Florence; Gerber-Lemaire, Sandrine; Schutz, Catherine; Vogel, Pierre
CORPORATE SOURCE: Institute of Chemical Sciences and Engineering, Swiss Federal Institute of Technology, EPFL-BCH, Lausanne, CH-1015, Switz.
SOURCE: Helvetica Chimica Acta (2004), 87(4), 800-810
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:38786

AB New 2-(aminomethyl)-5-(hydroxymethyl)pyrrolidine-3,4-diol derivs. were synthesized from (5S)-5-[(trityloxy)methyl]pyrrolidin-2-one and their inhibitory activities toward glycosidases were evaluated. The influence of the configuration of the pyrrolidine ring on glycosidase inhibition was evaluated. (2R,3R,4S,5R)-2-[(benzylamino)methyl]-5-(hydroxymethyl)pyrrolidine-3,4-diol was a good and selective inhibitor of α-mannosidase from jack bean (Ki = 1.2 μM) and from almond (Ki = 1.0 μM). Selectivity was lost for the non-benzylated derivative (2R,3R,4S,SR)-2-(aminomethyl)-5-(hydroxy-ethyl)pyrrolidine-3,4-diol which inhibited α-galactosidases, β-galactosidases, β-glucosidases, and α-N-acetylgalactosaminidase as well.

IT **704901-91-7P 704901-99-5P 704902-18-1P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(syntheses from (5S)-5-[(trityloxy)methyl]pyrrolidin-2-one and glycosidase inhibitory activities of 2-(aminomethyl)-5-(hydroxymethyl)pyrrolidine-3,4-diol derivs.)

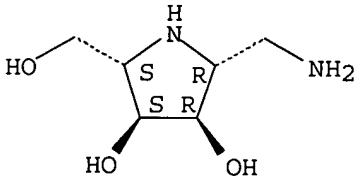
RN 704901-91-7 HCAPLUS
CN 3,4-Pyrrolidinediol, 2-(aminomethyl)-5-(hydroxymethyl)-, (2S,3S,4R,5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



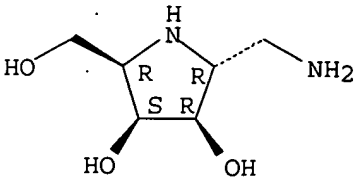
RN 704901-99-5 HCAPLUS
CN 3,4-Pyrrolidinediol, 2-(aminomethyl)-5-(hydroxymethyl)-, (2R,3R,4S,5S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



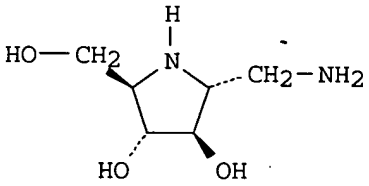
RN 704902-18-1 HCAPLUS
CN 3,4-Pyrrolidinediol, 2-(aminomethyl)-5-(hydroxymethyl)-, (2R,3R,4S,5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:330838 HCAPLUS
DOCUMENT NUMBER: 135:122363
TITLE: Powerful probes for glycosidases novel, fluorescently tagged glycosidase inhibitors
AUTHOR(S): Hermetter, Albin; Scholze, Hubert; Stutz, Arnold E.; Withers, Stephen G.; Wrodnigg, Tanja M.
CORPORATE SOURCE: Institut fur Biochemie der Technischen Universitat Graz, Graz, A-8010, Austria
SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(10), 1339-1342
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:122363
GI



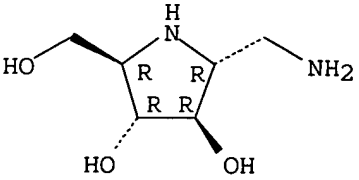
I

AB 1-Amino-1,2,5-trideoxy-2,5-imino-D-mannitol(I) was fluorescently tagged by reaction with dansyl chloride at N-1 or by attachment of a dansyl amide bearing spacer to this center. Compds. obtained are highly potent inhibitors of β-glucosidase exhibiting Ki values in the single figure nanomolar range. The 1-N-dansyl substituted inhibitor was successfully exploited for binding studies with β-glucosidase from Agrobacterium sp. employing fluorescence spectrometric methods.

IT **194288-65-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and evaluation of fluorescently tagged stereo-specific pyrrolidine derivs. as β-glucosidase inhibitors)

RN 194288-65-8 HCAPLUS
CN 3,4-Pyrrolidinediol, 2-(aminomethyl)-5-(hydroxymethyl)-, (2R,3R,4R,5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



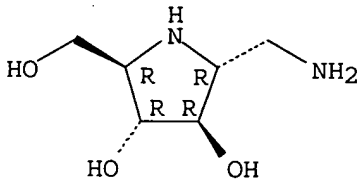
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:279046 HCAPLUS
DOCUMENT NUMBER: 135:133923
TITLE: Novel, lipophilic derivatives of 2,5-dideoxy-2,5-imino-D-mannitol (DMDP) are powerful β-glucosidase inhibitors
AUTHOR(S): Wrodnigg, T. M.; Withers, S. G.; Stutz, A. E.
CORPORATE SOURCE: Glycogroup, Institut fur Organische Chemie, Technische Universitat Graz, Graz, A-8010, Austria
SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(8), 1063-1064
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:133923

AB Novel derivs. of the d-glucosidase inhibitor 2,5-dideoxy-2,5-imino-D-mannitol bearing lipophilic aliphatic or aromatic amides attached to C-1 have been found to inhibit β-glucosidase from Agrobacterium sp. in the nanomolar range. One of them, a coumarin derivative, ranks amongst the most active compds. in the class of reversible glycosidase inhibitors of the iminoalditol type. Novel 1-N-acyl and 1-N-sulfonyl derivs. of 1-amino-1,2,5-trideoxy-2,5-imino-D-mannitol exhibiting Ki values in the nanomolar range are reported.

IT **194288-65-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and structure activity relations of novel, lipophilic derivs. of dideoxyiminomannitol as β-glucosidase inhibitors)
RN 194288-65-8 HCAPLUS
CN 3,4-Pyrrolidinediol, 2-(aminomethyl)-5-(hydroxymethyl)-, (2R,3R,4R,5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:787884 HCAPLUS
DOCUMENT NUMBER: 134:71810
TITLE: Biologically active 1-aminodeoxy and 1-O-alkyl derivatives of the powerful D-glucosidase inhibitor 2,5-dideoxy-2,5-imino-D-mannitol
AUTHOR(S): Wrodnigg, Tanja M.; Gaderbauer, Walter; Greimel, Peter; Hausler, Herwig; Sprenger, Friedrich K.; Stutz, Arnold E.; Virgona, Chris; Withers, Stephen G.
CORPORATE SOURCE: Glycogroup, Institut fur Organische Chemie, Technische Universitat Graz, Graz, A-8010, Austria
SOURCE: Journal of Carbohydrate Chemistry (2000), 19(8), 975-990

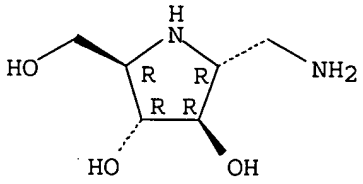
CODEN: JCACDM; ISSN: 0732-8303
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:71810

AB By an Amadori rearrangement of easily available 5-azido-5-deoxy-D-glucofuranose with dibenzylamine and subsequent catalytic hydrogenation of the resulting 5-azido-1-(N,N-dibenzyl)amino-1,5-dideoxy-D-fructopyranose, 1-amino-1,2,5-trideoxy-2,5-imino-D-mannitol was obtained in only two steps and in excellent overall yield. Likewise, other amines were employed to introduce extended side chains ultimately suitable for attachment of the inhibitor to solid supports. The reported rearrangement reaction is a high yielding, convenient and apparently general entry to 1-aminodeoxyketopyranoses modified at C-5, facilitated by the ring enlargement of the aldofuranose to the ketopyranose as an addnl. driving force. A range of selected chain extended analogs was prepared by acylation of N-1. Inhibitors obtained exhibit Ki-values with D-glucosidases in the micromolar range. Interestingly, 1-N-acylation resulted in superior inhibitory activities, as did the addition of a hexyl chain.

IT **194288-65-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of biol. active aminodeoxy and alkyl aminotrideoxyiminomannitol derivs. of the powerful D-glucosidase inhibitor 2,5-dideoxy-2,5-imino-D-mannitol)

RN 194288-65-8 HCAPLUS
CN 3,4-Pyrrolidinediol, 2-(aminomethyl)-5-(hydroxymethyl)-, (2R,3R,4R,5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:125861 HCAPLUS
DOCUMENT NUMBER: 132:237302
TITLE: Synthesis and evaluation as glycosidase inhibitors of 2,5-imino-D-glucitol and 1,5-imino-D-mannitol related derivatives
AUTHOR(S): McCort, Isabelle; Fort, Sebastien; Dureault, Annie; Depezay, Jean-Claude
CORPORATE SOURCE: Universite Rene Descartes, Laboratoire de Chimie et Biochimie Pharmacologiques et Toxicologiques, associe au CNRS, Paris, 75270, Fr.
SOURCE: Bioorganic & Medicinal Chemistry (2000), 8(1), 135-143
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Selectively functionalized 2,5-imino-D-glucitol and 1,5-imino-D-mannitol

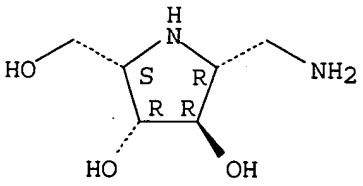
derivs. were synthesized and tested as precursors of hydrolytically resistant pseudo-disaccharides. Among them N-acetyl-6-amino-6-deoxy-2,5-imino-D-glucitol and N-acetyl-6-amino-6-deoxy-1,5-imino-D-mannitol were found to be potent and specific inhibitors against β-D-glucosidase and α-L-fucosidase, resp.

IT **194288-74-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and evaluation as glycosidase inhibitors of iminoglucitol and iminomannitol related derivs.)

RN 194288-74-9 HCAPLUS

CN 3,4-Pyrrolidinediol, 2-(aminomethyl)-5-(hydroxymethyl)-, (2R,3R,4R,5S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:358812 HCAPLUS

DOCUMENT NUMBER: 129:136393

TITLE: Synthesis of ester- and amide-linked pseudo-azadisaccharides via coupling of D-glucose with 6-amino-6-deoxy-2,5-imino-D-glucitol

AUTHOR(S): McCort, Isabelle; Dureault, Annie; Depezay, Jean-Claude

CORPORATE SOURCE: Laboratoire de Chimie et Biochimie Pharmacologiques et Toxicologiques associe au CNRS, Universite Rene Descartes, Paris, 75270, Fr.

SOURCE: Tetrahedron Letters (1998), 39(25), 4463-4466
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Hydrolytically-resistant pseudodisaccharides incorporating an azafuranose have been prepared by coupling 6-amino-2,5-imino-D-glucitol derivs. with D-glucose, either through an ester or an amide bond. Synthesis of the azasugar templates was achieved by nucleophilic opening of a C2 sym. bis-aziridine deriving from D-mannitol.

IT **210479-79-1P 210479-81-5P 210479-83-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of ester- and amide-linked pseudoazadisaccharides via coupling of glucose with aminodeoxyiminoglucitol)

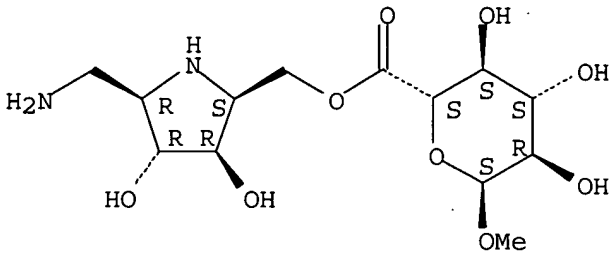
RN 210479-79-1 HCAPLUS

CN α-D-Glucopyranosiduronic acid, methyl, [(2S,3R,4R,5R)-5-(aminomethyl)-3,4-dihydroxy-2-pyrrolidinyl]methyl ester, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

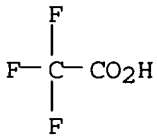
CRN 210479-78-0
CMF C13 H24 N2 O9

Absolute stereochemistry. Rotation (+).



CM 2

CRN 76-05-1
CMF C2 H F3 O2

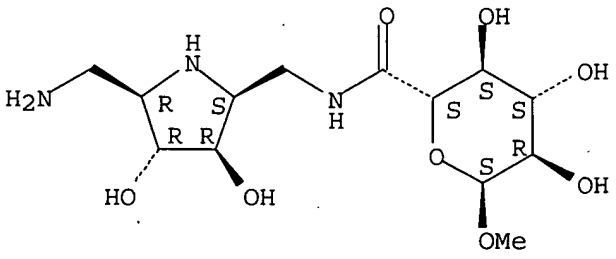


RN 210479-81-5 HCAPLUS
CN α-D-Glucopyranosiduronamide, methyl N-[[(2S,3R,4R,5R)-5-(aminomethyl)-3,4-dihydroxy-2-pyrrolidinyl]methyl]-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 210479-80-4
CMF C13 H25 N3 O8

Absolute stereochemistry. Rotation (+).



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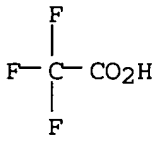
CRN 76-05-1
CMF C2 H F3 O2

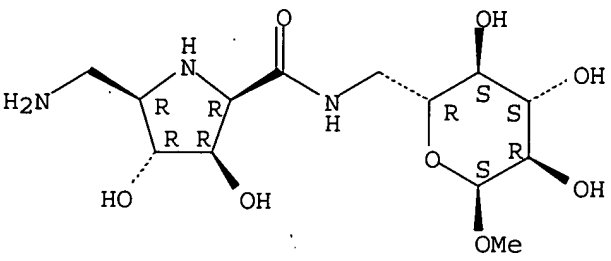


RN 210479-83-7 HCAPLUS
CN α-D-Glucopyranoside, methyl 6-[[[(2R,3R,4R,5R)-5-(aminomethyl)-3,4-dihydroxy-2-pyrrolidinyl]carbonyl]amino]-6-deoxy-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

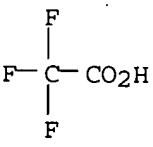
CRN 210479-82-6
CMF C13 H25 N3 O8

Absolute stereochemistry. Rotation (+).



CM 2

CRN 76-05-1
CMF C2 H F3 O2



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

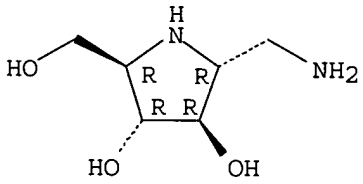
L4 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:530913 HCAPLUS
DOCUMENT NUMBER: 127:190944
TITLE: Synthesis of 1-amino-1,2,5-trideoxy-2,5-imino-D-mannitol, a novel analog of the powerful glucosidase inhibitor 2,5-dideoxy-2,5-imino-D-mannitol, via an Amadori rearrangement of 5-azido-5-deoxy-D-glucofuranose
AUTHOR(S): Wrodnigg, Tanja M.; Stutz, Arnold E.; Withers, Steven G.

CORPORATE SOURCE: Institut fur Organische Chemie der Technischen Universitat Graz, Graz, A-8010, Austria
SOURCE: Tetrahedron Letters (1997), 38(31), 5463-5466
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB By an Amadori rearrangement of easily available 5-azido-5-deoxy-D-glucofuranose with dibenzylamine and subsequent catalytic hydrogenation of the resulting 5-azido-1-dibenzylamino-1,5-dideoxy-D-fructopyranose, the new 1-amino-1,2,5-trideoxy-2,5-imino-D-mannitol was obtained in only two steps and excellent overall yield. Likewise, other amines and/or other 5-modified hexofuranoses can be used to advantage. The reported rearrangement reaction is a high yielding, convenient and apparently general entry to 1-aminodeoxyketopyranoses modified at C-5, facilitated by the ring enlargement of the aldofuranose to the ketopyranose as an addnl. driving force.

IT **194288-65-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aminotrideoxyiminomannitol via an Amadori rearrangement of azidodeoxyglucofuranose)
RN 194288-65-8 HCAPLUS
CN 3,4-Pyrrolidinediol, 2-(aminomethyl)-5-(hydroxymethyl)-, (2R,3R,4R,5R)-(9CI) (CA INDEX NAME)

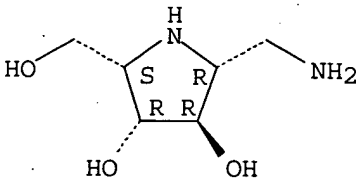
Absolute stereochemistry. Rotation (+).



10L (b)

IT **194288-74-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of aminotrideoxyiminomannitol via an Amadori rearrangement of azidodeoxyglucofuranose)
RN 194288-74-9 HCAPLUS
CN 3,4-Pyrrolidinediol, 2-(aminomethyl)-5-(hydroxymethyl)-, (2R,3R,4R,5S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:433855 HCAPLUS

DOCUMENT NUMBER: 122:291430
TITLE: Synthesis and Evaluation of Homoaza Sugars as Glycosidase Inhibitors
AUTHOR(S): Wong, Chi-Huey; Provencher, Louis; Porco, John A., Jr.; Jung, Sang-Hun; Wang, Yi-Fong; Chen, Lihren; Wang, Ruo; Steensma, Darryl H.
CORPORATE SOURCE: Department of Chemistry, Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Journal of Organic Chemistry (1995), 60(6), 1492-501
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
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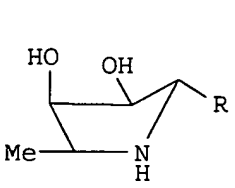

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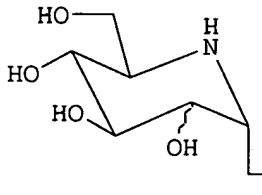

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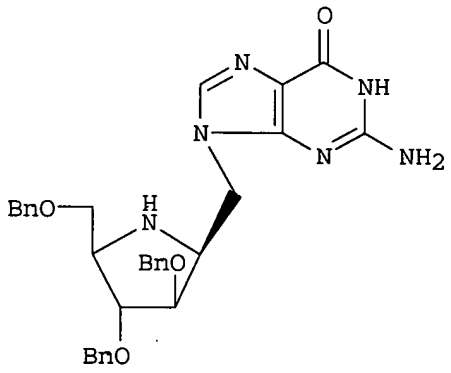


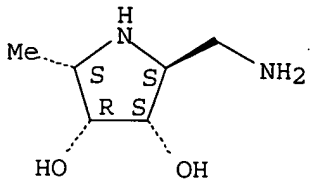
III

AB In an effort to develop transition-state mimetics of the glycosidase-catalyzed reaction, five- and six-membered azasugars and their homo-analogs were prepared and tested as inhibitors of glycosidases. Inhibition studies indicate that the fucosyl cation-like, five-membered imine and its reduced form I (R = H) are potent inhibitors of α-fucosidase from bovine kidney with resp. Ki values of 160 nM and 2 μM. The five-membered homoaminoaza sugar I (R = CH2NH2) is also a potent inhibitor of the enzyme (Ki = 1.9 + 10-6 M), while the glucose and mannose-like six-membered homoaminoaza sugars II are less potent than the corresponding 1-deoxyaza sugars as inhibitors of α-glucosidase and α-mannosidase, resp. The primary amino group was placed in an attempt to introduce addnl. electrostatic interactions in the active site. The inhibitory activities are, however, in the high μM range. Synthesis of homoaza sugars structurally related to a disaccharide and a nucleoside III is also described.

IT **162895-60-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and evaluation of homoaza sugars as glycosidase inhibitors)
RN 162895-60-5 HCAPLUS
CN 3,4-Pyrrolidinediol, 2-(aminomethyl)-5-methyl-, monohydrochloride, [2S-(2α,3β,4β,5β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

L4 ANSWER 11 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1991:101739 HCAPLUS
DOCUMENT NUMBER: 114:101739
TITLE: Preparation of heterocyclic medical chelating agents and chelates
INVENTOR(S): Almen, Torsten; Berg, Arne; Dugstad, Harald; Klaveness, Jo; Krautwurst, Klaus Dieter; Rongved, Pal
PATENT ASSIGNEE(S): Cockbain, Julian Roderick Michaelson, UK; Nycomed A/S
SOURCE: PCT Int. Appl., 53 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9008138	A1	19900726	WO 1990-EP79	19900115
W: AU, CA, FI, GB, JP, NO, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE				
CA 2045539	AA	19900714	CA 1990-2045539	19900115
AU 9049573	A1	19900813	AU 1990-49573	19900115
AU 646795	B2	19940310		
EP 452392	A1	19911023	EP 1990-901813	19900115
EP 452392	B1	19950412		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE				
JP 04502619	T2	19920514	JP 1990-502171	19900115
JP 2953670	B2	19990927		
AT 121079	E	19950415	AT 1990-901813	19900115
ES 2071089	T3	19950616	ES 1990-901813	19900115
NO 9102749	A	19910712	NO 1991-2749	19910712
NO 177783	B	19950814		
NO 177783	C	19951122		
FI 96416	B	19960315	FI 1991-3388	19910712
FI 96416	C	19960625		
US 5348954	A	19940920	US 1991-690975	19910724
US 5439668	A	19950808	US 1994-235882	19940502
PRIORITY APPLN. INFO.:			GB 1989-719 A	19890113
			WO 1990-EP79 A	19900115

US 1991-690975 A3 19910724

OTHER SOURCE(S): MARPAT 114:101739

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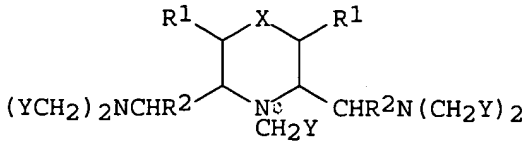

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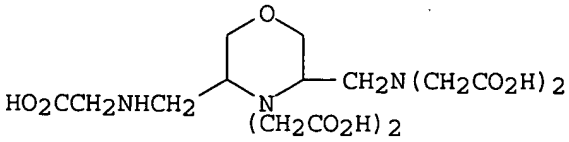


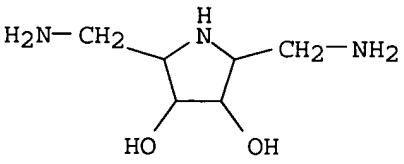
II

AB Title compds. I [X = bond, O, S, R1HC, R3N, R1, R2 = H, (substituted) alkyl, alkoxyalkyl; R3 = H, mono-, polyhydroxylated alkyl, etc.; Y = hydroxycarbamoyl, COZ; Z = (substituted) morpholino, etc.] useful as diagnostic, therapeutic, detoxification, imaging, or radiotherapy agents (no data), are prepared Thus, title compound II, prepared starting from 3-carboxamido-5-cyano-4-benzylmorpholine via 3,5-bis(aminomethyl)morpholine, was reacted with Gd2O3 in the presence of NaOH to give the 2Na salt of the Gd(III) chelate of II. Pharmaceutical formulations containing I salts and chelates are given.

IT **131883-77-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of medical chelating agent)

RN 131883-77-7 HCAPLUS

CN 3,4-Pyrrolidinediol, 2,5-bis(aminomethyl)-, trihydrochloride (9CI) (CA INDEX NAME)



●3 HCl

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	73.94	235.48

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	ENTRY	SESSION
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DICTIONARY FILE UPDATES: 30 NOV 2005 HIGHEST RN 869059-01-8

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TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

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* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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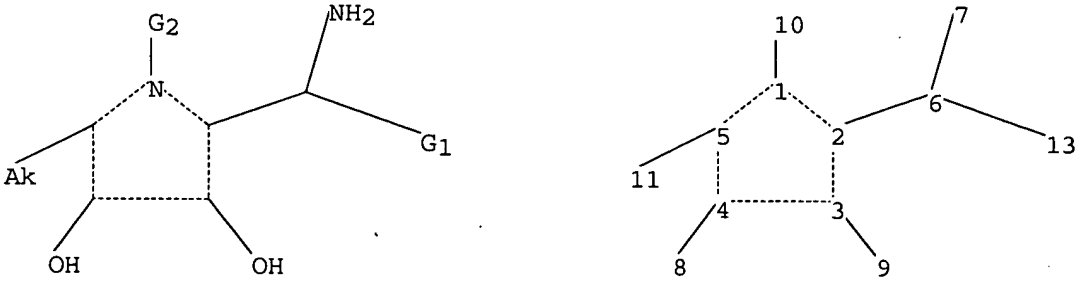

chain nodes :
6 7 8 9 10 11 13
ring nodes :
1 2 3 4 5
chain bonds :
1-10 2-6 3-9 4-8 5-11 6-7 6-13

ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-10 2-3 3-4 3-9 4-5 4-8 5-11 6-7 6-13
exact bonds :
2-6
isolated ring systems :
containing 1 :

G1:H,CH2,COOH

G2:C,CH3

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 13:CLASS

L5 STRUCTURE UPLOADED

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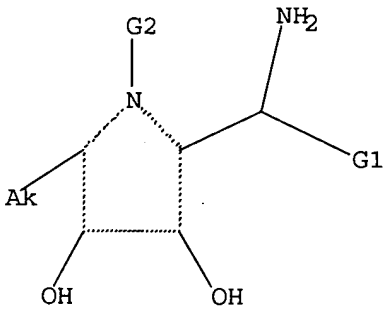
L5 HAS NO ANSWERS
L5 STR



G1 H,CH2,COOH
G2 C,Me

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 68 TO ITERATE

100.0% PROCESSED 68 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 866 TO 1854
PROJECTED ANSWERS: 0 TO 0

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SEARCH TIME: 00.00.01

L7             1 SEA SSS FUL L5

=> FIL HCAPLUS
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CA SUBSCRIBER PRICE                                     0.00      -8.03

FILE 'HCAPLUS' ENTERED AT 13:18:40 ON 02 DEC 2005
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FILE COVERS 1907 - 2 Dec 2005  VOL 143 ISS 24
FILE LAST UPDATED: 1 Dec 2005  (20051201/ED)

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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> S L7
L8             1 L7

=> d l8 ibib abs hitstr tot

L8   ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         1995:994843  HCAPLUS
DOCUMENT NUMBER:          124:117885
TITLE:                    Preparation of 2-chloro and 2-bromo derivatives of
                          1,5-iminosugars as glycosidase inhibitors and
                          intermediates.
INVENTOR(S):              Barta, Thomas E.; Mueller, Richard A.
PATENT ASSIGNEE(S):       G.D. Searle and Co., USA
SOURCE:                   PCT Int. Appl., 92 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
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LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9524392	A1	19950914	WO 1995-US2168	19950228
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TT, UA				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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AU 9519258	A1	19950925	AU 1995-19258	19950228
US 5595981	A	19970121	US 1995-399022	19950306
US 5612480	A	19970318	US 1995-398839	19950306
US 5663342	A	19970902	US 1996-663507	19960614
PRIORITY APPLN. INFO.:			US 1994-207340 A	19940308
			WO 1995-US2168 W	19950228
			US 1995-399022 A1	19950306

OTHER SOURCE(S): MARPAT 124:117885
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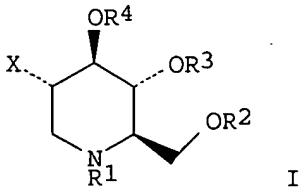
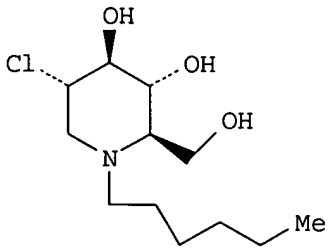


I



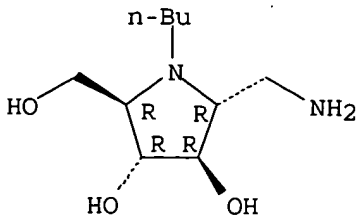
II

AB Title compds. [I; X = Cl, Br; R1 = H, C1-12 (branched) alkyl, alkoxyalkyl, alkenyl, alkynyl, (substituted) aralkyl, aralkenyl; R2-R4 = H, COR5; R5 = C1-6 (branched) alkyl, C6-12 aryl, alkylaryl], were prepared Thus, title compound (II), prepared from N-hexyldeoxynojirimycin, inhibited HIV with EC50 = 11 μg/mL.

IT **172936-42-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-chloro and 2-bromo derivs. of 1,5-iminosugars as glycosidase inhibitors and intermediates)

RN 172936-42-4 HCAPLUS
CN 3,4-Pyrrolidinediol, 2-(aminomethyl)-1-butyl-5-(hydroxymethyl)-, [2R-(2α,3β,4α,5β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	7.39	404.20

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.73	-8.76

STN INTERNATIONAL LOGOFF AT 13:19:11 ON 02 DEC 2005